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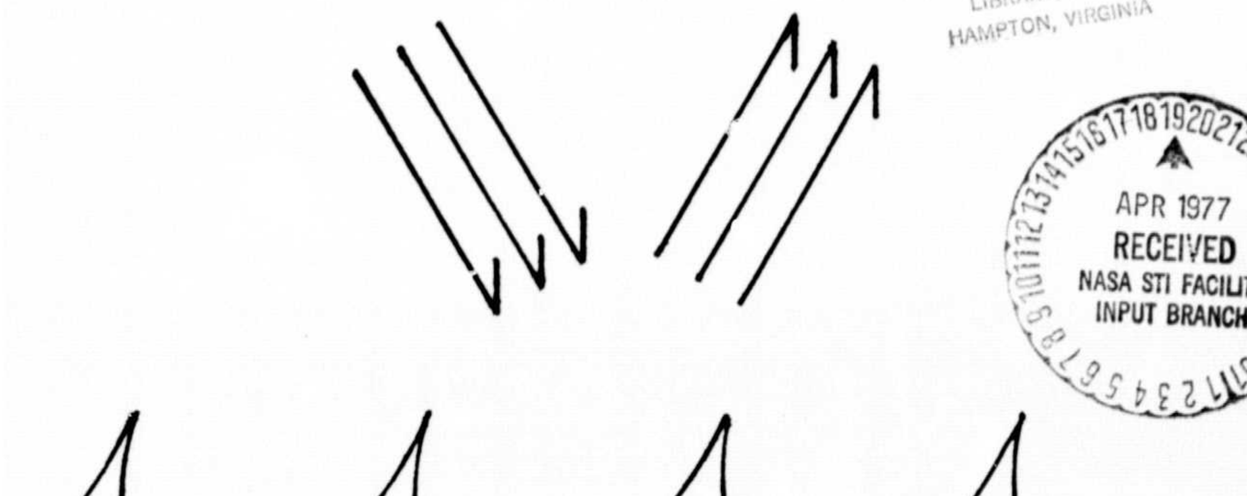
REMOTE SENSING OF CHLOROPHYLL CONCENTRATION STATE-OF-THE-ART - 1975

by

B.H. Atwell

JANUARY 1976

Report No. 156



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ABSTRACT

Remote measurement of chlorophyll concentration of the world's oceans from satellite observations could potentially be extremely useful for assessments of productivity in large areas for which measurements by other means would be impractical.

The basis of these measurements rests with the physics of the interaction of light with material dissolved and suspended in the water. It is possible theoretically to predict the nature of light upwelled from the ocean surface from a solution to the radiative transfer equation. Practically, however, this is difficult. Monte-Carlo methods presently are thought to be the most viable method to treat the general theoretical problem. With restrictive assumptions of the nature of scattering, it is possible to construct simpler models.

Due to complications inherent in the theoretical approach, many purely empirical studies have been conducted. From these, algorithms have been developed which successfully relate chlorophyll concentration (or some other parameter, i.e., seechi depth) to the upwelled light spectrum. A common shortcoming of these studies is that none of them have shown the algorithm developed to have general applicability, or provide an indication of the limits of conditions for which the algorithm is useful.

INTRODUCTION

Within the last decade, development of aircraft and satellite remote sensing technology has made possible observations of the oceans on a spatial scale heretofore unavailable. Analysis techniques for data collected are presently being developed. One area of study which has received a good deal of interest is the assessment of chlorophyll content from measurements of water color. This paper is designed to provide the reader with a summary of the status of these studies at present.

The chlorophylls are a group of plant pigments. These pigments have the ability to absorb solar radiation and to use this energy in the photosynthetic cycle of the plant. A number of chlorophylls have been recognized and have been termed a, b, c, d, and e. Chlorophyll a is present in all plants and is the pigment which gives them their characteristic green color. It is the most abundant of all the chlorophylls. The other chlorophylls are accessory pigments and may or may not be present in a given plant type. Chlorophyll measurements provide an estimate of primary productivity within a given oceanic area. These measurements on a periodic basis would provide a much better understanding than that which now exists about primary production in vast areas of the world oceans. Potentially, this could have far-reaching effects on fisheries resource assessment and the conduct of ocean fisheries.

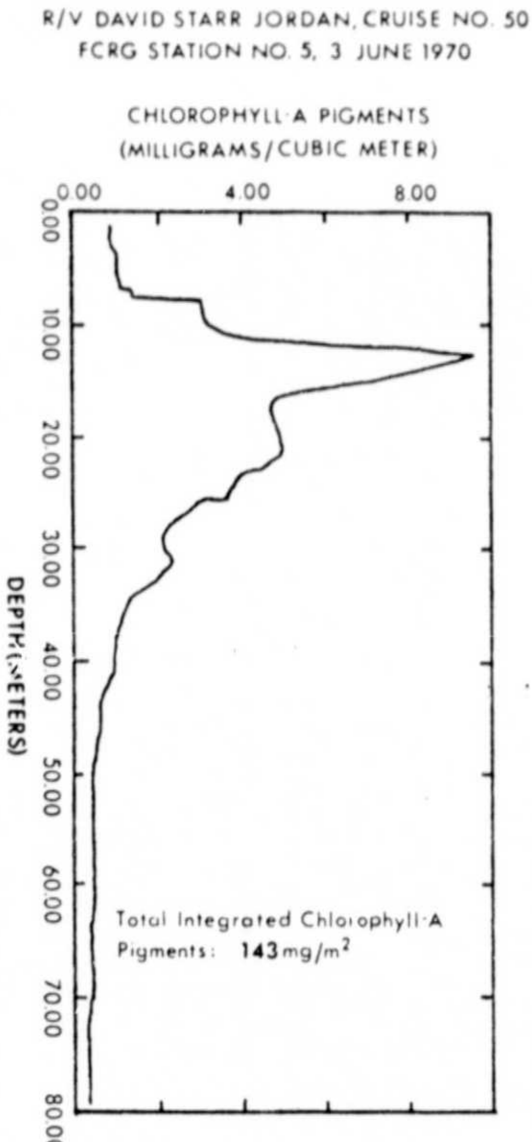
CHLOROPHYLL IN SEA WATER

Although all plants contain chlorophyll, attempts at remote measurement of chlorophyll in the marine environment have been directed toward measuring chlorophyll contained in phytoplankton as opposed to larger rooted plants which exist in shallow water. The horizontal distribution of phytoplankton in the oceans is controlled to a large degree by the availability of nutrients. Areas of sustained high productivity exist only in regions where nutrients are continuously supplied, i.e., areas of large scale upwelling where nutrient rich bottom water is brought to the surface. The other factor which enters into the rate of production of phytoplankton production is of course the availability of light.

In much of the worlds oceans the rate of phytoplankton production shows large seasonal variation (Ryther, 1959). Generally, there is a short period of peak production which is many times the annual mean. Within a given region, the horizontal distribution of phytoplankton often has a "patchy" nature. Thus, at any given instance in time, there may be both large and small scale horizontal variations in the distribution of phytoplankton.

Phytoplankton are not distributed vertically in any predictable pattern. Duntley, et al.,(1974) refer to depth profiles of chlorophyll a collected by the Food Chain Research Group of the Institute of Marine Resources, University of California, stating that the curves from many different ocean areas were very diverse, showing nearly every conceivable distribution save one-- one which was constant with depth. Typical examples are shown in Figure 1.

The upwelled light at the surface is affected by materials within the entire euphotic zone; however, intuitively one would expect the near surface chlorophyll to exert a disproportional effect. This was confirmed by modeling (Duntley, et al., 1974). Moreover, these models predicted diffuse spectral reflectance curves for chlorophyll distributions of Figure 1, which show a threefold variation in total chlorophyll, to be almost identical in the green and depart only slightly in the blue and red. Even in these regions of the



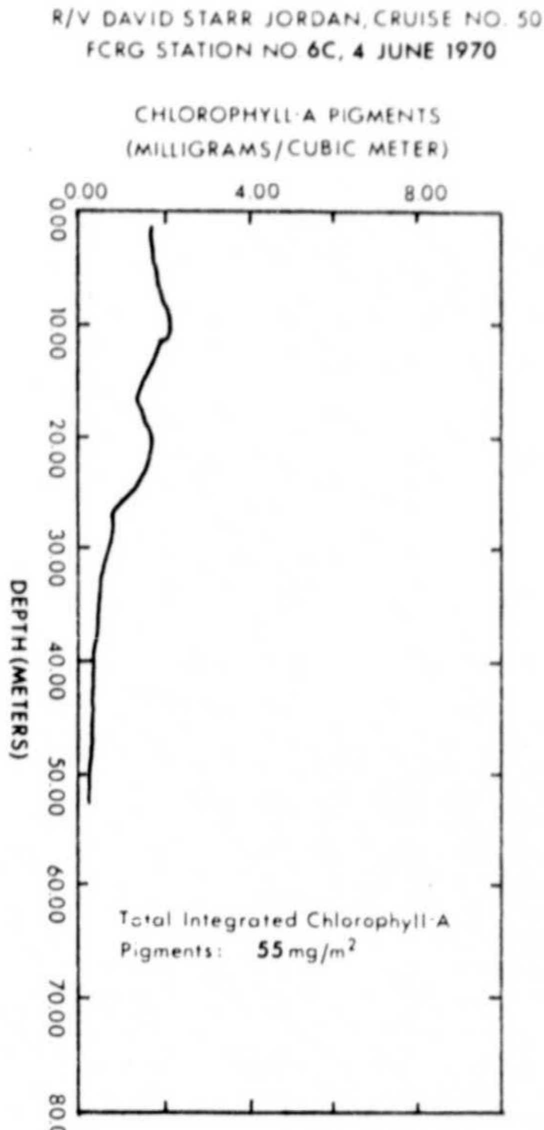


Fig. 1. Chlorophyll-A Pigment Depth Profiles measured in situ in waters near San Diego. (From Research on the Marine Food Chain Progress Report, July 1970 - June 1971, Institute of Marine Resources, Report 71-10, Part III Data Records.)

spectrum the change was contrary to what would be expected for a homogenous distribution. The model based on the highest total chlorophyll (Figure 2, Station 5) showed higher reflectance in the blue and lower in the red, just opposite to what would normally be expected. Before leaving this topic, Duntley's (1974) conclusion should be stated: "Thus, the subsurface spectral diffuse reflectance is wholly ambiguous as a measure of total chlorophyll _a_ pigments present, even to a spectroradiometer located just below the water surface." This statement has strong implications to the entire study of remote chlorophyll measurement. At the very least, it indicates that efforts to relate _surface_ measurements of chlorophyll to the upwelled reflectance spectrum are ill-advised. Some early investigations (Clark, _et al._, 1970; Weldon, 1973, etc.) were based on relations with surface measurements and have indicated reasonable correlations. This could have been due to looking at grossly different water types as was the case with Clark, _et al._, or perhaps by making measurements in shallow, well-mixed water as was the case with Weldon.

Investigators other than Duntley have realized the vertical distribution of chlorophyll exerts an important effect on the upwelling radiation. Mueller (1973) discusses this problem in some detail and concludes that some depth weighted value is required. He derives from considerations of a two flow radiative transfer model what he defines as the net equivalent color concentration (NECC), and successfully correlates spectral response to the parameter.

INTERACTION OF LIGHT AND WATER

Natural light impinging on the water surface is of two forms - the direct collimated rays of the sun and diffuse light from the sky. The light is partitioned at the water surface, part is transmitted into the water, and the

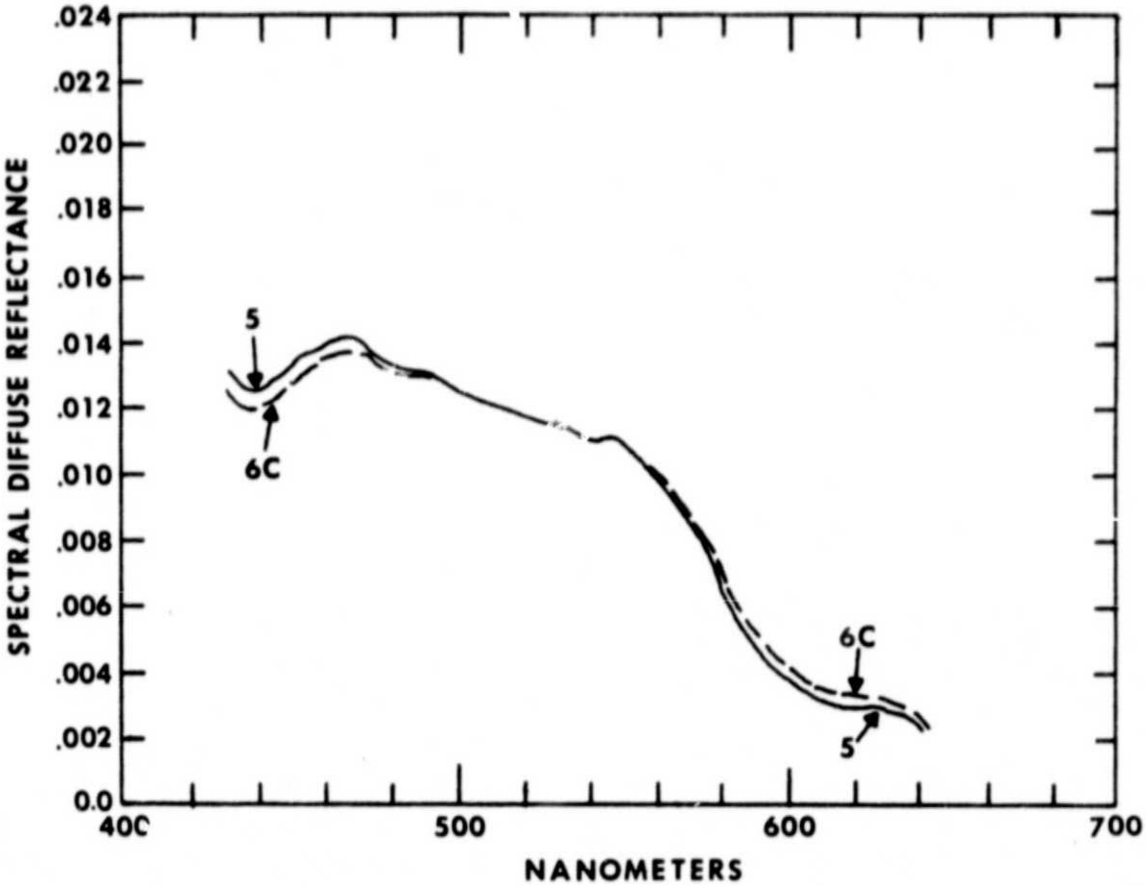


Fig. 2. Subsurface spectral diffuse reflectance at Station 5 (solid line) and Station 6C (dashed line). (From Duntley <u>et al</u>. 1974.)

remainder is reflected. Light entering the water is scattered and absorbed by the water molecules and dissolved and suspended material. A part of this light is backscattered toward the air-water interface where it is again partially reflected and transmitted. That portion which is transmitted through the air-water interface contains information about the water constituents and is the part which is of interest in determining characteristics of water remotely. An understanding of the relationship between water characteristics and upwelling light is only possible through consideration of all the factors influencing it--reflection, scattering, and absorption.

Reflection

Partitioning of energy of direct rays of the sun, assuming an optically flat water surface, can be predicted from Fresnel's equation:

$$\frac{(Is)_r}{Is} = {}^1/_2 \left[\frac{\tan^2 (\alpha-\beta)}{\tan^2 (\alpha+\beta)} + \frac{\sin^2 (\alpha-\beta)}{\sin^2 (\alpha+\beta)} \right]$$

α = Zenith distance of the sun

β = Angle of refraction between water and air

Jerlov (1968) includes a table of $\frac{(Is)_r}{Is}$ as a function of zenith distance. For values from 0 to 45° the reflection ranges from 2% to 2.8%; as the angle increases past 45° reflection increases rapidly up to 100% at 90°. Reflection of the diffuse light from the sky can be determined by integration of the Fresnel equation over the sky hemisphere. This has been done by several investigators. Burt (1954) summarizes this research and quotes a consistent value of 6.6%. Preisendorfer (1957) computed a value of 5.2% for a cardioid distribution of sky radiation. Thus, a value of 5% to 6% for sky reflection seems well established.

Fresnel's equation applies to reflection from a flat surface. The sea surface, of course, is not flat; so it is of interest to determine how the roughness of the sea surface changes the reflectivity. Cox and Munk (1956) consider the effect of a roughed sea surface on reflection. Their analysis demonstrates that direct reflection of the sun is independent of wave conditions for solar zenith angles of less than 20°, increases for angles 20 - 60°, and decreases for angles greater than 60° (Figure 3). For sky light, a decrease in reflectance of about 1% for a rough sea versus a smooth sea was observed.

Albedo of Sea Surface

The albedo of the sea surface is the percent of incident energy which is upwelled from the surface. It is important to note that this includes both light reflected from the surface and that backscattered from within the water.

Clarke and Ewing (1973) present their estimate of a typical ocean and Albedo model (Figure 4). A basic assumption of this model is that most of the energy reaching the surface comes directly from the sun; thus the contribution due to skylight was neglected. According to this model, emergent backscattered light which contains information regarding water constituents makes up 25% of the total upwelling light and 0.5% of the total incident light.

Absorption

The absorption properties of distilled water show that an absorption minimum occurs at 460 nm (Figure 5). Jerlov (1968) cites the research of Clarke and James (1939) and Sullivan (1963) as evidence that sea salts exert little influence on the absorption qualities of sea water; thus, the absorption

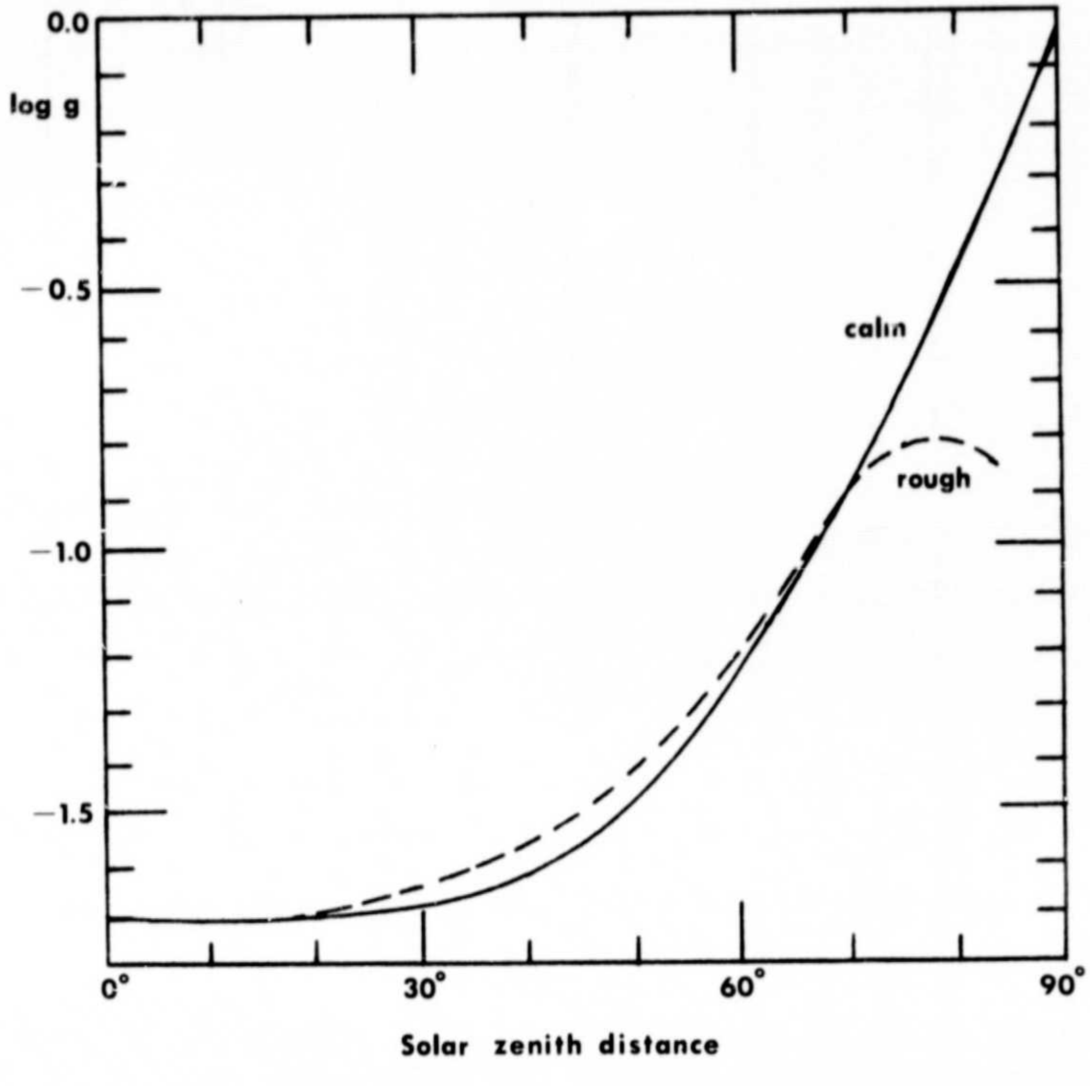


Fig. 3. Reflectance of solar radiation from a flat surface and from a surface roughened by a Beaufort 4 wind. (After COX and MUNK, 1956.)

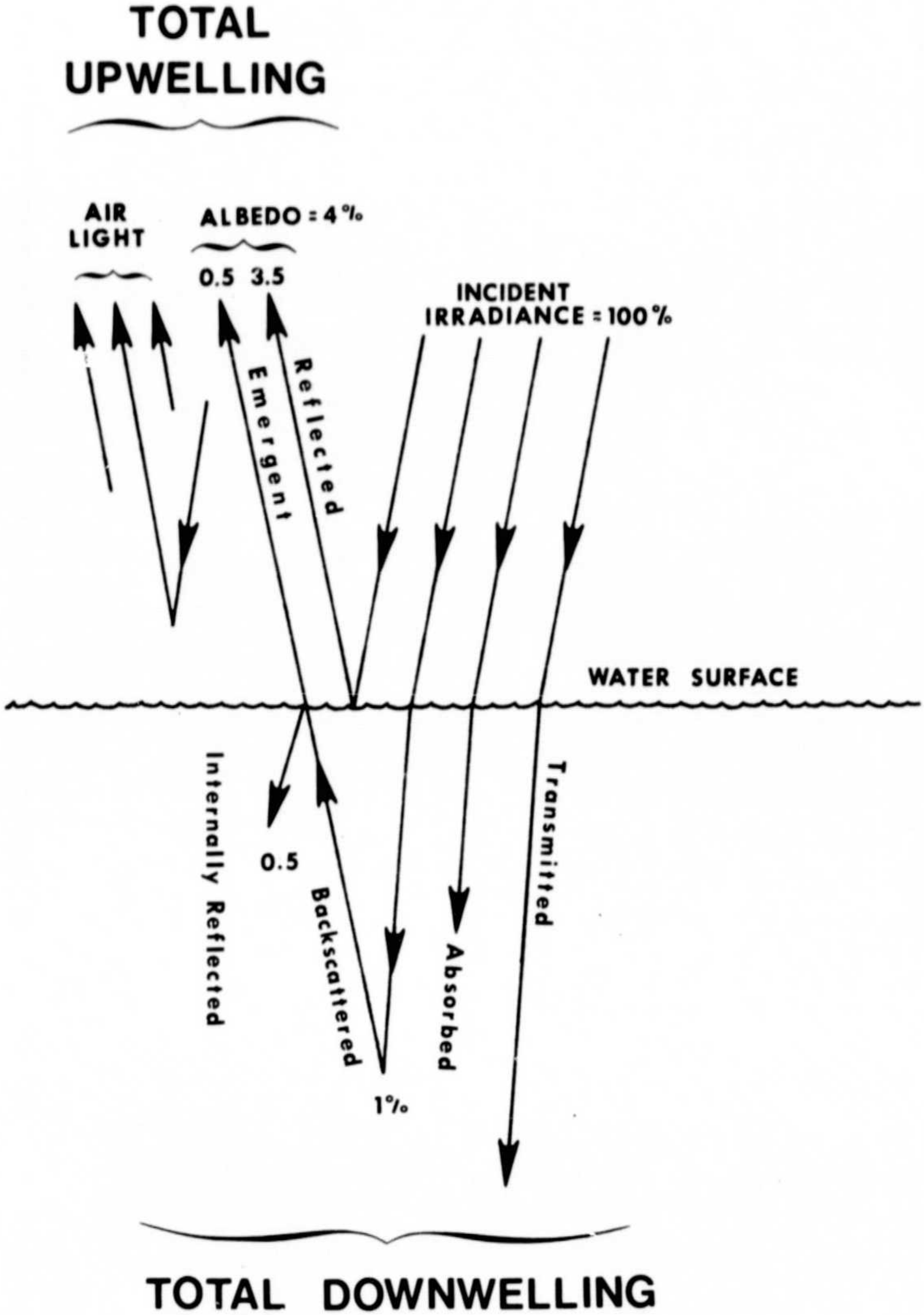


Fig. 4. Schematic representation of the fate of the incident radiation in the air above the surface of the sea, at the surface itself, and in the water beneath the surface. The percentages are based on the findings of Payne (1971) for conditions at the entrance of Buzzards Bay, Mass.

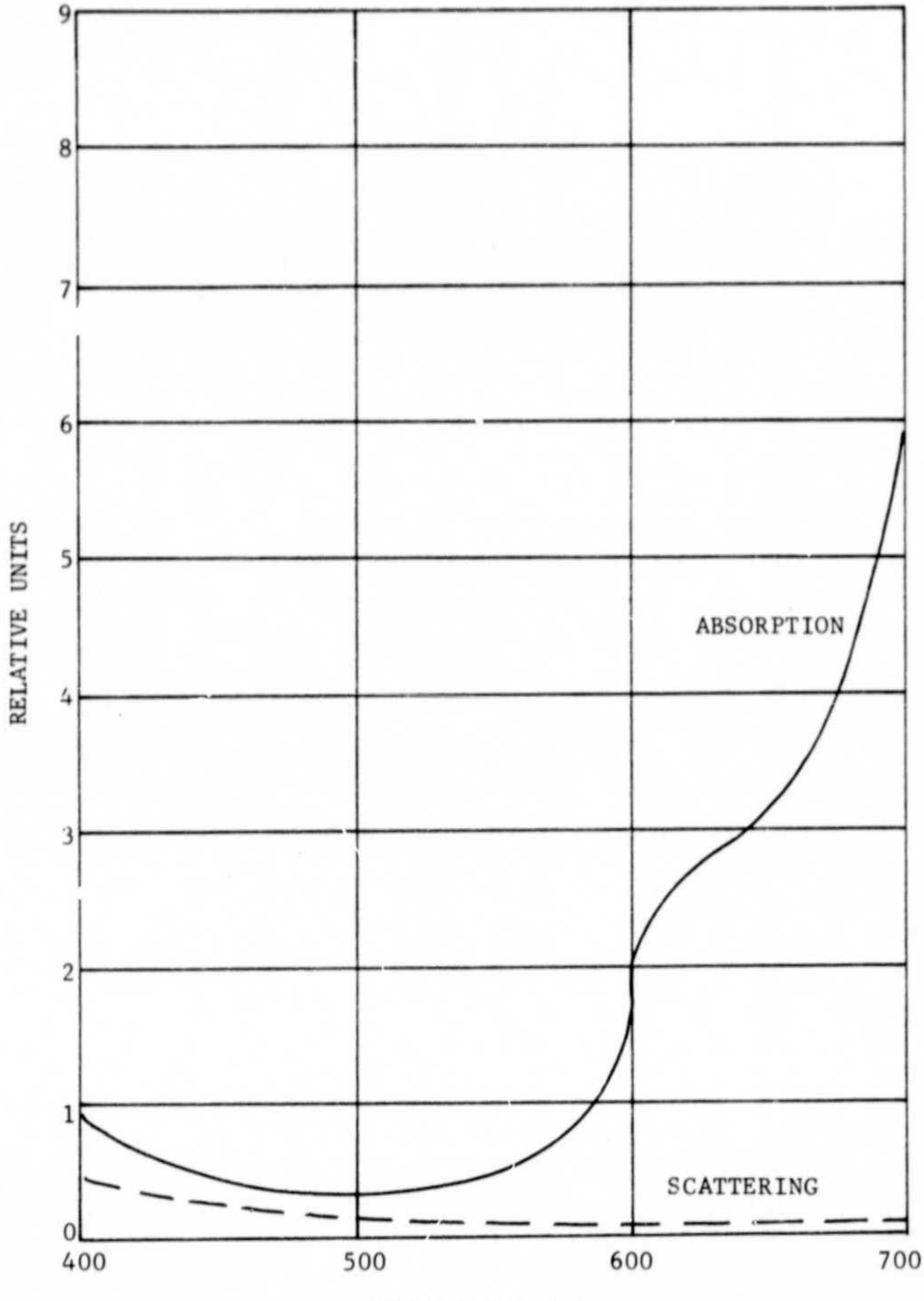


Figure 5. Absorption and Scattering of Distilled Water. (After Hulbert, 1945.)

of pure sea water should be identical with that of distilled water. An important factor in absorption qualities of sea water is the so-called "yellow substances." Attention was called to these by Kalle (1938), and they have been the object of considerable research since that time (Kalle, 1962, 1966). For our purposes, let it suffice to say that they are a complex group of soluble organic compounds common to most marine waters, and they are thought to exert, because of their distinctive absorption characteristics, a significant influence on water color. The "yellow substances" absorb most strongly in the ultra-violet and blue regions, having little effect in the red (Figure 6).

Absorption of light by particulate material suspended in the water was studied by Burt (1958). Burt obtained absorption measurements of filtered sea water and assumed that these were the combined effect of water and dissolved materials. He subtracted this from attenuation of the unfiltered samples and deduced that the residual effect was due to particulate matter (Figure 7). Assuming that scattering is independent of wavelength, higher attenuation at the shorter wavelengths is thought due to absorption by particles.

Scattering

Scattering by pure water has been shown generally to be in accord with molecular scattering theory developed by Rayleigh (1871). This theory predicts scattering will be proportional to the inverse of the fourth power of the wavelength; thus, shorter wavelengths will undergo more scattering than the longer. Jerlov (1968) suggests that scattering in water is more accurately described by the fluctuation theory proposed by Smoluchowski (1908) and Einstein (1910). A modification of the formula proposed by Einstein has

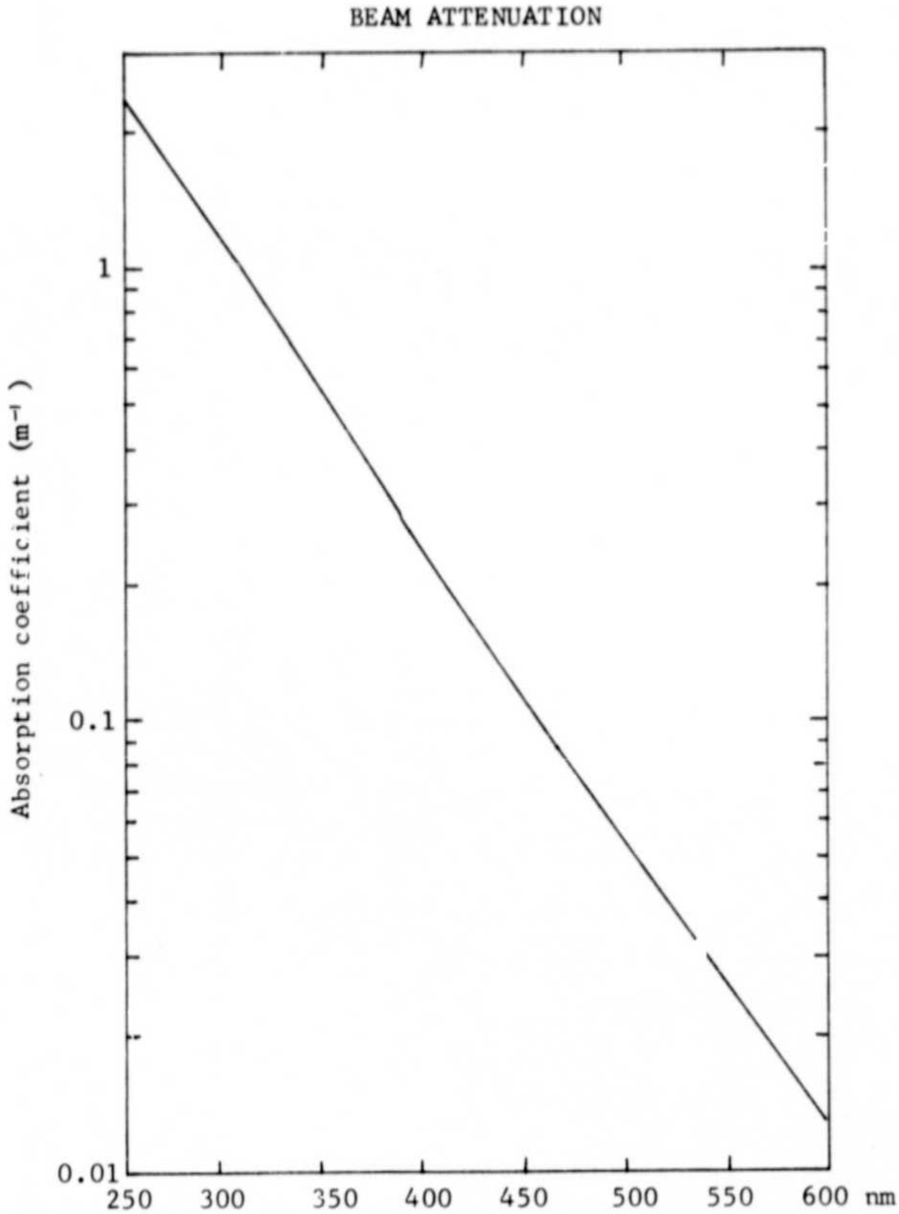


Fig. 6. Absorption curve for yellow substance. (From Jerlov, 1968.)

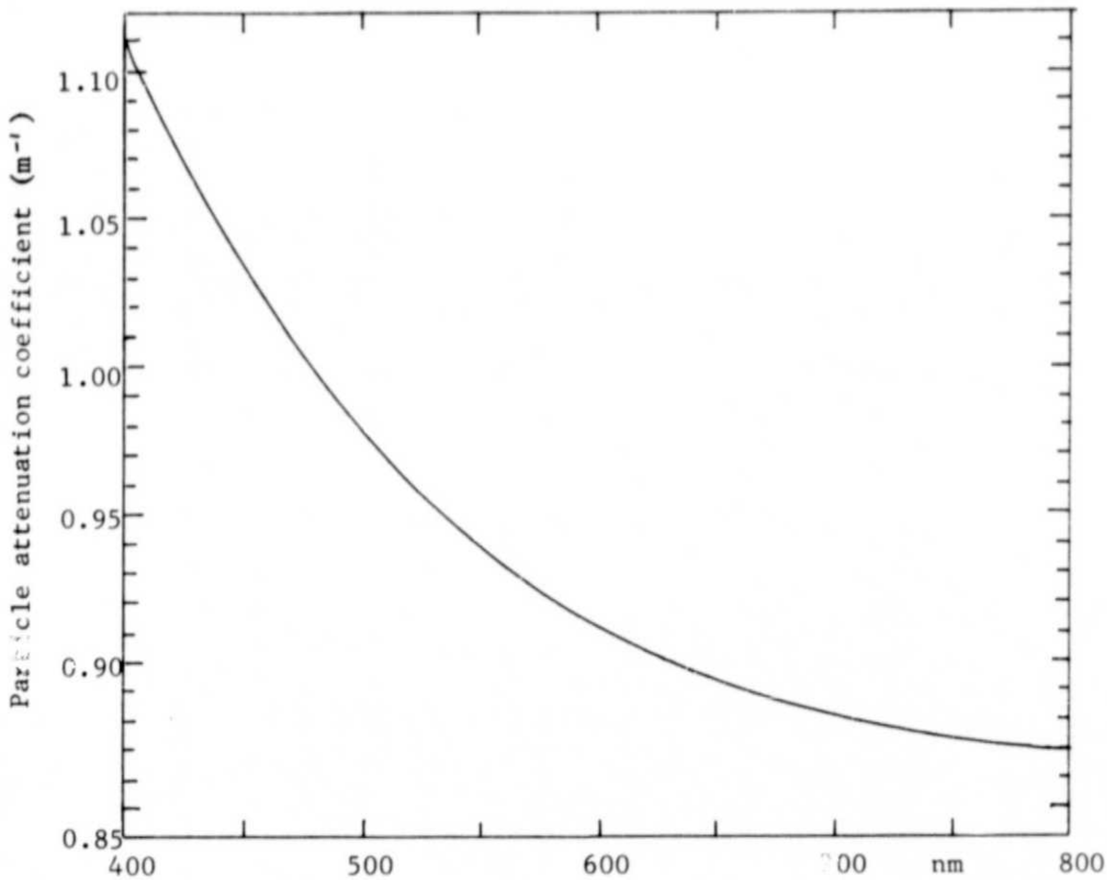


Fig. 7. Light attenuance caused by particulate matter. (After Burt, 1958.)

been shown to provide the closest agreement with experimental values (Peyrot, 1938). Morel (1966) conducted experiments which further verified the λ^4 relationship and showed the effect of dissolved sea salts to be very small.

The physical processes involved in particle scattering are reflection, refraction, and diffraction of light by the particles. Development of a theory which accurately accounts for these phenomena is understandably complex. Mie (1908) treated the problem of scattering from a monochromatic plane wave by nonabsorbing spherical particles using electromagnetic theory. He derived expressions for the intensity of scattered light in the planes perpendicular and parallel to the plane of observation i_1 and i_2, respectively. The physical parameters which enter into these functions are the diameter of the particle, wavelength of the incident wave, and the refractive index of the particle relative to the surrounding medium. From Mie's theory a quantity of light scattered in the direction (Θ) from a randomly polarized beam of unit intensity will be (Jerlov, 1968):

$$i\ (\Theta) = \frac{\lambda^2}{8\pi^2}(i_1 + i_2)$$

The total light scattered may be obtained by integrating the above equation.

$$I = 2\pi \int_o^{\pi} i(\Theta) \sin\Theta d\Theta$$

$$= \frac{\lambda^2}{4\pi} \int_o^{\pi} (i_1 + i_2) \sin\Theta d\Theta$$

Dividing the total scattered light by the cross sectioned area of the particle results in a dimensionless quantity K called the efficiency factor or effective area coefficient:

$$K = \frac{4I}{\pi D^2} = \frac{\lambda^2}{\pi^2 D^2} \int_o^{\pi} (i_1 + i_2)\sin\theta d\theta$$

Theoretical treatment (Burt, 1956) and experiments (Hodkinson, 1963; Jerlov and Kullenberg, 1953) have shown that the value of K approaches 2 for particles greater than 1μ in diameter.

Particle scattering obtained from measurements from which scattering due to water has been subtracted has shown that particle scattering in many diverse types of water is similar (Figure 8). In all cases, there was strong forward scattering.

OPTICAL PROPERTIES OF PHYTOPLANKTON-CHLOROPHYLL

A much referred to study by Yentsch (1960) provides the absorption spectra for several different species of phytoplankton (Figure 9). The absorption of all these species is greatest in the blue and red portion of the spectrum with minimum absorption in the green. Yentsch also computed curves showing the combined absorption of both chlorophyll and water for different concentration of chlorophyll (Figure 10). It is apparent from this figure that water tends to decrease the prominence of absorption in the red portion of the spectrum. Little difference is seen in absorption of red light for chlorophyll concentration of less than 3 mg/m^3. For this reason, much subsequent research in the remote sensing of chlorophyll has been directed toward making these measurements in the blue portion of the spectrum. It would seem possible, however, that the red portion might be useful for high concentrations.

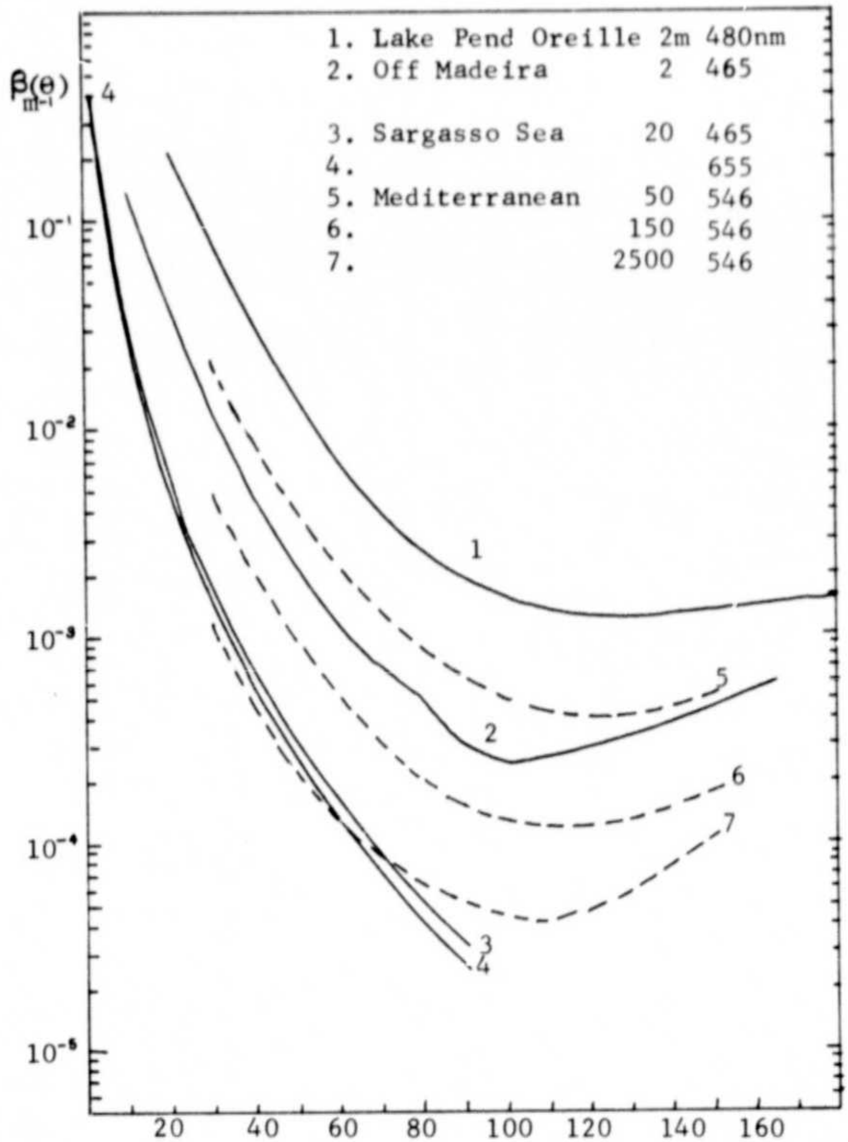


Fig. 8. Particle scattering functions obtained by deducting the theoretical function for pure water from functions observed in the Mediterranean (sample 5-7; Morel, 1966), in the Sargasso Sea (3, 4; Kullenberg, 1966), off Madeira (2; Jerlov, 1961), and in Lake Pend Oreille (1; Tyler, 1961a).

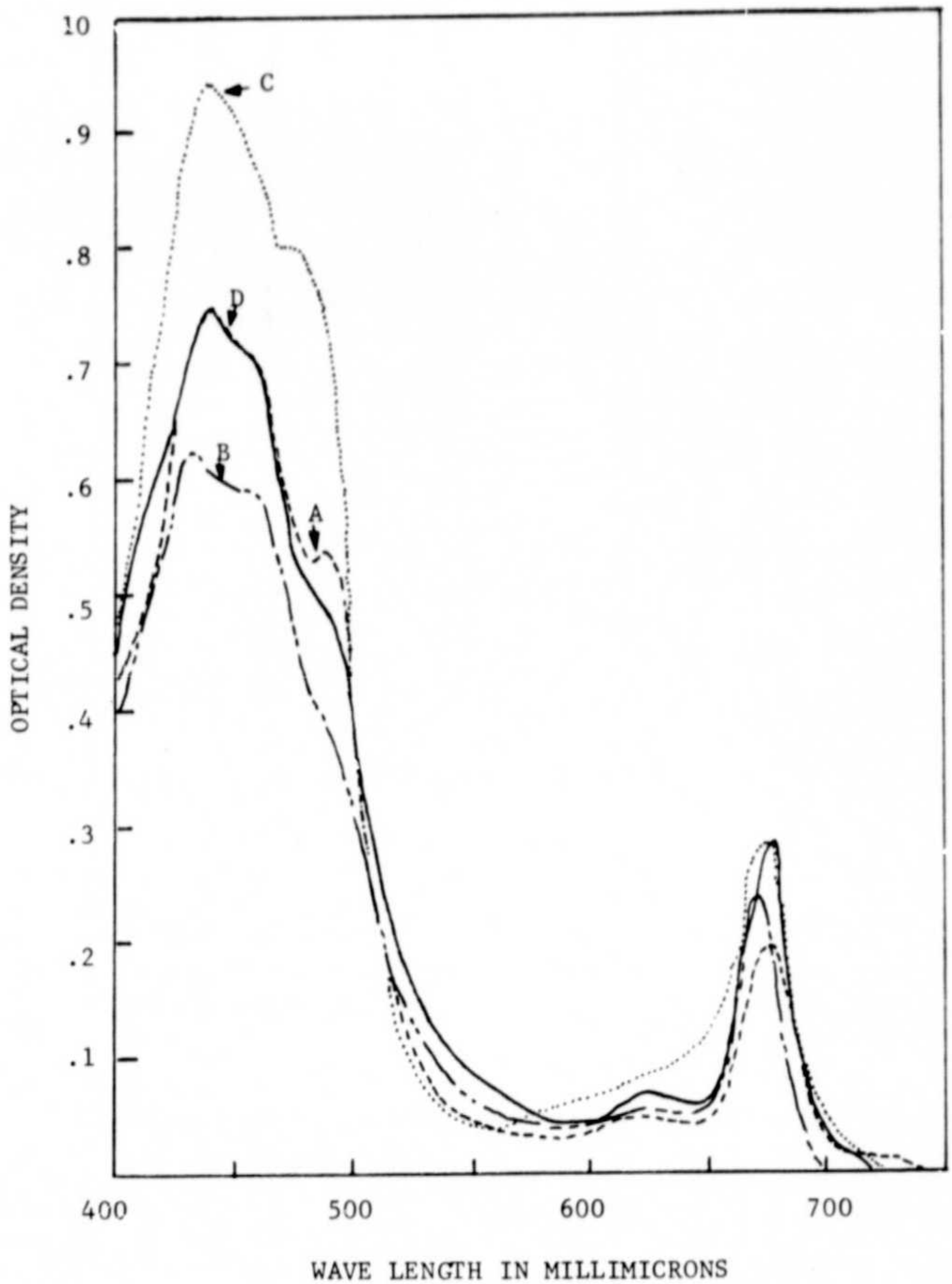


Fig. 9. Pigment spectra of living phytoplankton, A. Diatom Cyclotella sp., B. Dinoflagellate, Amphidium sp., C. green Flagellate Chlamydomonas, D. Natural population sampled from Woods Hole waters. (From Yentsch, 1959.)

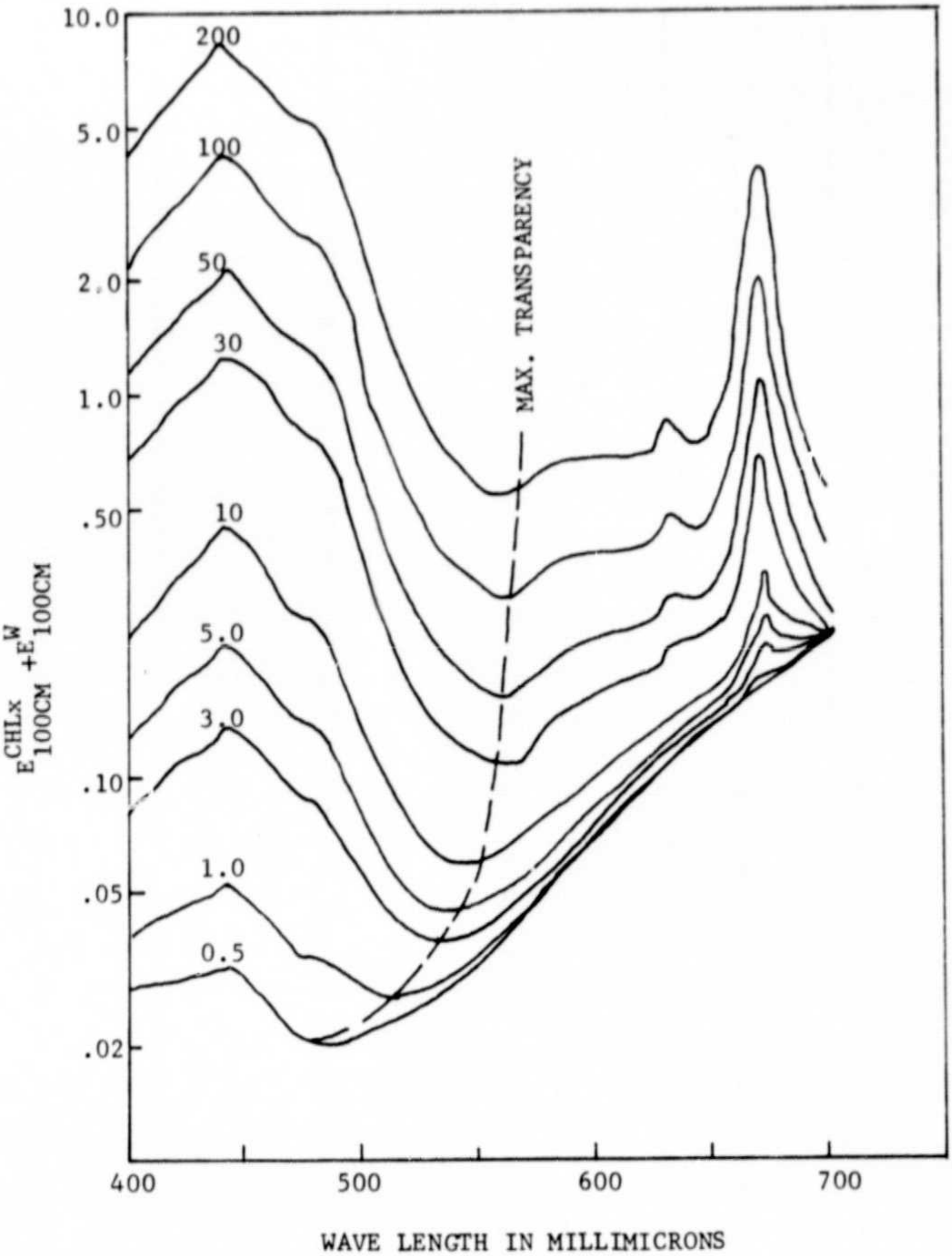


Fig. 10. Combined absorption coefficients for pure water and plant pigments. Numbers adjacent the curves indicate the chlorophyll concentration in mgs./m^3. (From Yentsch, 1959.)

Ramsey (1968) combined the research of Yentsch with that of Hulbert (1943, 1945) to derive theoretical reflectance curves for a deep ocean, a sunny day, a solar zenith angle of 45° and homogenous chlorophyll concentrations varying from 0 to 100 mg/m^3 (Figure 11). As would be expected, curves corresponding to low chlorophyll concentrations have high reflectance in the blue and low in the green. The curves for high chlorophyll are exactly opposite. Reflectance appears to be little affected by chlorophyll concentration at wavelengths around 0.5 micron. Strong red absorption of chlorophyll was evident for chlorophyll concentrations greater than 10 mg/m^3.

Mueller (1973) challenged the assumption that an accurate description of the interaction with light with phytoplankton could be obtained by combining the absorption of extracted chlorophyll with white scattering due to plant cells. He supported this hypothesis by Mie theory calculation which indicated the scattering of light by spherical cells simulating photoplankton is wavelength dependent.

EXPERIMENTAL REMOTE SENSING STUDIES

Clarke, Ewing, and Lorenzen (1970) showed that the percent of incident light backscattered (that portion upwelling from the surface) could be related to chlorophyll concentration. Measurements were made along a profile extending from the east U. S. coast to the Sargasso Sea. Surface truth measurements indicated there was a continual decrease in chlorophyll concentration along that transect, which is also evidenced by the spectra measured from the aircraft (Figure 12). The author noted that an inverse relationship existed between the mean slope of the spectra and the chlorophyll content. Percent reflectance for curves B, C, and E, corresponding to surface truth measurements

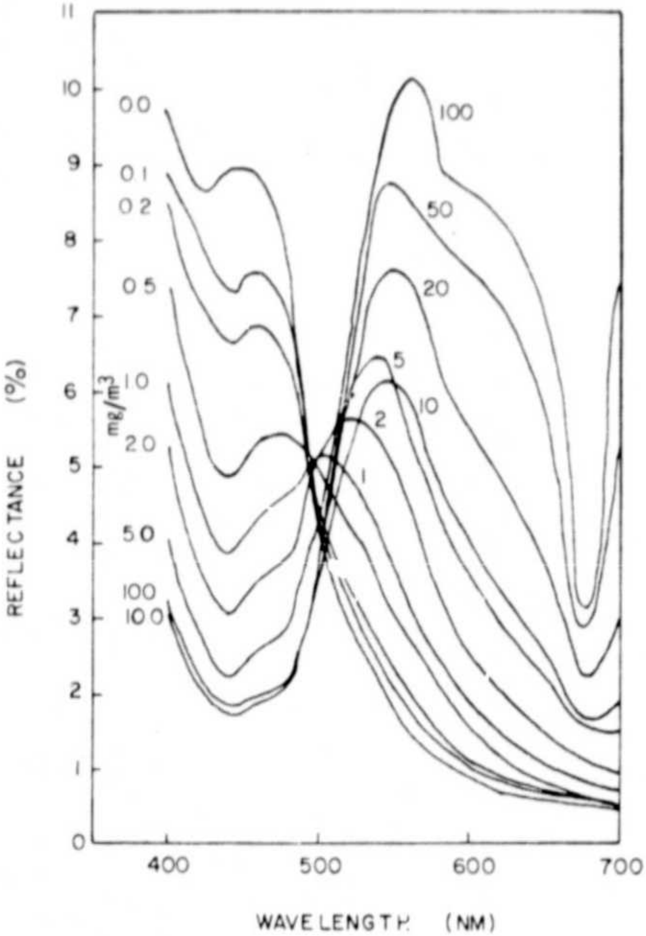


Fig. 11. Spectral reflectance of sea water for several different concentrations of chlorophyll (mg/m^3), as calculated with Hulburt's (1943) equations. (After Ramsey, 1968.)

OCEAN COLOR DETECTION

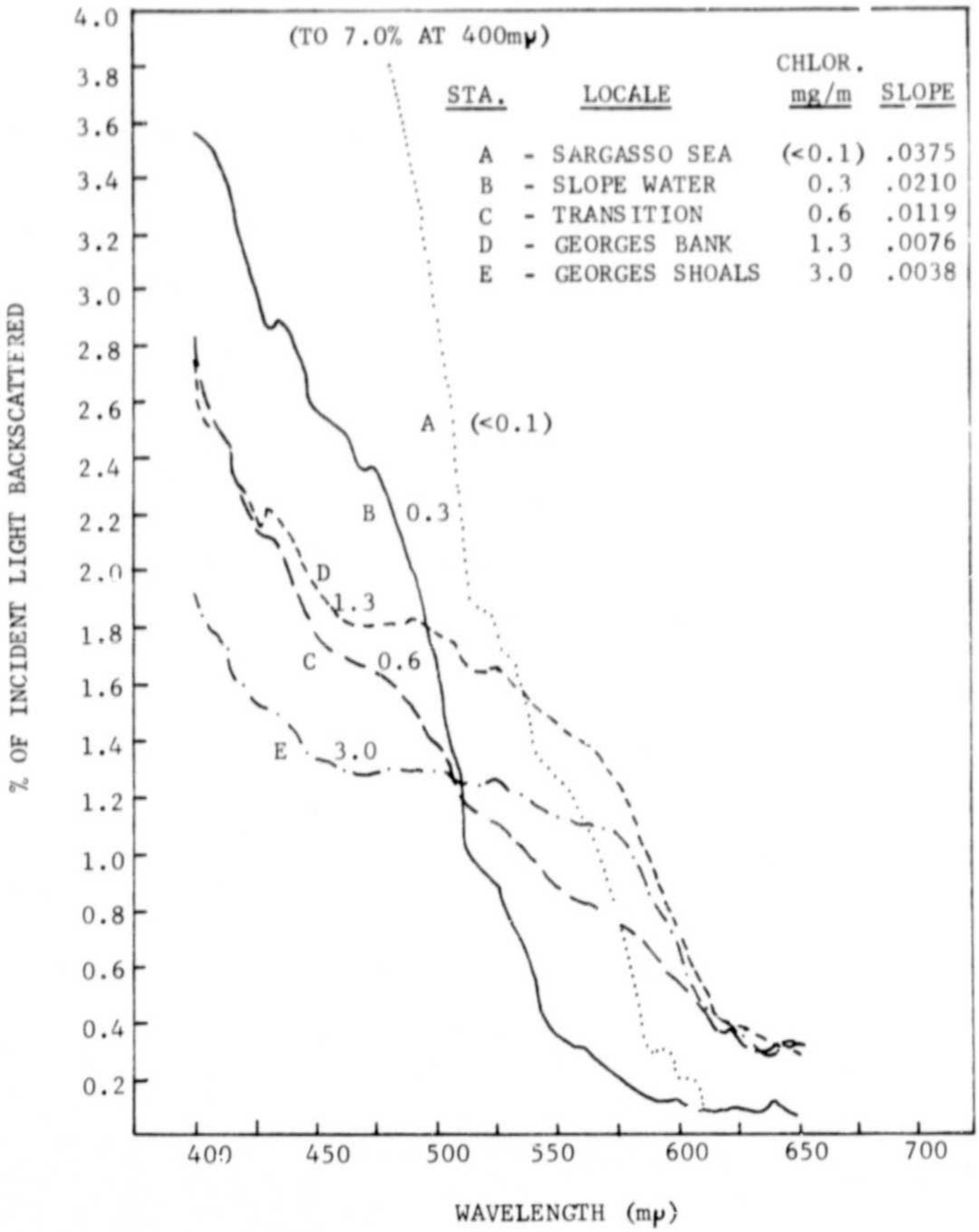


Fig. 12. Spectra of backscattered light measured from the aircraft at 305m on 27 August 1968 at the following stations and times (all E.D.T.): Station A, 1238 hours; Station B, 1421 hours; Station C, 1428.5 hours; Station D, 1445 hours; Station E, 1315 hours. The spectrometer with polarizing filter was mounted at 53° tilt and directed away from the sun. Concentrations of chlorophyll a were measured from shipboard as follows: on 27 August, Station A, 1238 hours; on 28 August, Station B, 060_ hours; Station C, 0730 hours; Station D, 1230 hours, (After Ewing, 1971.)

of 0.3, 0.6 and 3.0 mg/m^3 of chlorophyll, respectively, were about the same at 515 nanometers. This corresponds well to a value of about 500 nanometers as predicted by Ramsey (1968). Considering the uncertainties involved in these measurements, particularly in the time and location compatibility between spectra and surface truth, the correlation between surface and remote measurements is surprisingly good.

Mueller (1973) made aircraft spectral measurements similar to those of Clarke et al. (1970). Comparison of his measurements with surface measurements of chlorophyll showed that significant changes in the spectra could be associated with changes in chlorophyll content. He realized that qualitative comparison of spectra left something to be desired as an analysis technique and cited Semenchenko (1967), Clarke et al. (1970), and Arvesen et al.(1971) as examples of possible ways to parameterize the spectral data. Respectively, they developed an algorithm to correlate radiances measured at 4 different wavelengths with Secchi-depth, related slope of spectra to chlorophyll content, and indicated that a correlation exists between chlorophyll concentration and the ratio of radiance at wavelengths of 443 and 525 nm. Mueller felt a weakness of all these techniques was the loss of spectral information as a result of parameterization. In order to avoid this, Mueller used an eigenvector or principal component analysis to parameterize his data. This technique is used to reduce the dimensionability of a set of data by transforming it into a second set with reduced dimensions but which contains essentially all the information of the original set. Mueller reduced a sample of 31 spectra to 1 mean vector M_j and four eigenvectors e_{ij}, where $i = 1, 2, 3, 4$ (index for each eigenvector) and $j = 1, 2, \ldots. 55$ (values of the variables of 55 different wavelengths). The principal components Y_i ($i = 1, 2, 3, 4$) which are associated with each of the original spectra are formed from:

$$Y_i = \sum_{j=1}^{55} e_{ij} (R_j - M_j) \quad i = 1, 2, 3, 4$$

Mueller determined that the first four eigenvectors accounted for 99% of the total sample variance, and the first two account for more than 95%.

These principal components were then related to chlorophyll concentration and Secchi extinction depth by using multiple linear regression analysis. From this algorithms were developed relating chlorophyll and Secchi extinction depth to the principal components associated with each of the individual spectra.

RADIATION MODELS

Prediction of light spectra upwelling from a water surface with defined illumination, surface characteristics, and concentrations of dissolved and suspended material may be accomplished through the construction of radiation models. Such models in theory could be used to associate a given observed spectra to certain types and amounts of water constituents. Aside from this, they may also be used to establish the lower bounds on concentrations of materials which could be determined from upwelled spectra, and they should generally contribute to a better understanding of the processes involved in the interaction of light with water.

Construction of a radiation model requires consideration of three separate problems (four, if the atmosphere is considered): first, the specular reflection of the sun and sky from the water surface; second, the effects of absorption by the water molecules and dissolved material; and third, scattering and absorption by particulates. The reflectance of the sun and sky can be treated using Fresnel's equation if the roughness of the sea surface is neglected.

Cox and Munk (1956) have shown that the change in reflection due to surface roughness is not so great as to make an assumption of a plane surface untenable, certainly not as a first step.

Absorption by the water itself and dissolved materials present less difficulty from a modeling point of view than the particulates (McCluney, 1974). Thus, the most significant part of the modeling problem is associated with the scattering and absorption of particulate material. Scattering and absorption within the water are described by the radiance transfer equation:

$$(1) \quad \frac{dL\ (Z,\ \Theta,\ \phi)}{dr} = -C(Z)\ L(Z,\ \Theta,\ \phi) + L^*\ (Z,\ \Theta,\ \phi)$$

where L = Radiance

$C(Z) = a(Z)+b(Z)$ = Total attenuation coefficient

$a(Z)$ = Absorption coefficient

$b(Z)$ = Scattering

L^* = Path function

The first term represents the loss by attenuation and the second the gain by scattering.

Prieur and Morel (1973) summarize solutions to the radiation transfer equation. There is no closed solution except in the one dimensional case. Most general solutions are complex mathematically and accounting for the air-sea interface would make them even more so. Because of this, Monte Carlo models appear at this time to be the most viable approach to detailed radiation transfer models for the oceans. Gordon and Brown (1973) using an approach similar to that of Plas and Kattawar (1972) have developed a Monte Carlo model for the oceans which has shown to agree with experimental measurements.

McCluney (1974) modified the single scattering theory proposed by Jerlov to include the effects of sky radiation and has made the assumption that no downwelling or forward scattering light is lost from the incident sunlight and skylight as they propagate downward in the sea. This quasi-single scattering model has been shown to agree well with results from the Monte Carlo model developed by Gordon and Brown. This model, as the Monte Carlo model, depends on experimentally determined optical properties.

Mueller (1973) transformed the single scattering model (Jerlov, 1968) into a vector space defined by the first four eigenvectors e_{ij} determined from observed ocean spectra. With this model he calculated reflectance spectra by varying independently the concentration of phytoplankton pigment, nonabsorbing particles, and yellow substances. In addition he calculated the effect of different scattering angles. These calculations indicated that concentration of phytoplankton was the major source of variation in ocean color. Particle concentration and yellow substance were also significant, but changes in scattering angle had little effect.

SUMMARY

Remote measurement of the upwelling light from natural water offers a method to survey large areas quickly and economically. The upwelling light (or color) is, neglecting effects of the bottom in shallow water, controlled by materials suspended and dissolved within the water. Thus, it would seem possible to infer something about the contents of water from its color. Certainly the development of such a technology seems feasible.

Reflection, scattering, and absorption of the incident light from the sun and sky are the processes by which a particular water color is developed. These processes are individually complex, and determining theoretically how they combine to form a given water color is a difficult undertaking. One way to circumvent this difficulty is to conduct empirical studies which consist of developing correlations between simultaneous remote and conventional measurements. Some of these studies have shown that the water color could be related to chlorophyll content. However, none has provided a technology which could be extended with confidence to other areas or times. Nevertheless, the internal consistency of these studies has been encouraging. The lack of knowledge concerning fundamental optical properties of water with varying amounts and types of suspended materials has been a detriment to the development of a universally applicable technology. Research into these areas is presently being conducted and within the next few years answers to these basic questions should provide a foundation for the development of a more meaningful technology.

In order to provide for an efficient and orderly conduct of water color studies within NASA an outline (NASA Outline for Water Color Studies) has been developed to guide research efforts at NASA centers.

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